

# Prospects for Quantum Simulations of the Strong Coupling Expansion

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in collaboration with

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Based on arXiv: 2406.18721, 2308.03196, 2412.11677, 2303.01467, 2212.11328

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## Sign Workshop

Bern, Jan. 21, 2025



# Outline

## Context:

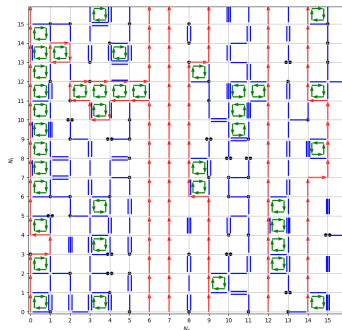
- Dual representation with staggered fermions: **effective theory of lattice QCD**
- Allow simulations at finite temperatures and densities
- Strong coupling expansion re-introduces sign problem, limiting range of validity
- Hamiltonian formulation based on dual representation may solve sign problem in quantum simulations

## Content of the talk:

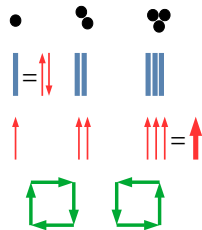
- 1 Monte Carlo simulations in dual representation including  $\mathcal{O}(\beta^2)$
- 2 SC-LQCD on the Quantum Annealer
- 3 Hamiltonian approach to strong coupling lattice QCD and its generalizations
- 4 Towards quantum computing: strategies and prospects

# Dual Representation of Lattice QCD

- For "standard" QCD lattice action (staggered fermions, Wilson gauge action)
- But: **change order of integration:**
  - expand in  $\beta = \frac{2N_c}{g^2}$
  - gauge links  $\{U_\mu(x)\}$  first
  - afterwards the quarks  
→ **no fermion determinant**
- "Dual" representation: via **color singlets!**
  - At  $\beta = 0$ : link states are **mesons** and **baryons** [Rossi, Wolff, NPB 248 (1984)]
  - At  $\beta > 0$ : color singlets may include gluons [Gagliardi, U, PRD 101 (2020)]
- Dual degrees of freedom:
  - monomers  $m_x$ : quark on site, weights for quark mass
  - dimers  $k_\mu(x)$ : mesons hoppings (quark-anti-quark pairs)
  - fermion world-lines  $f_\mu(x)$ : quark hoppings, weights depend on chemical potential, form closed loops
  - plaquette occupation numbers  $n_p, \bar{n}_p$ : expansion order from gauge action



2-dim. example of configuration in terms of dual variables

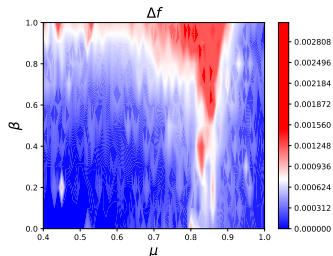
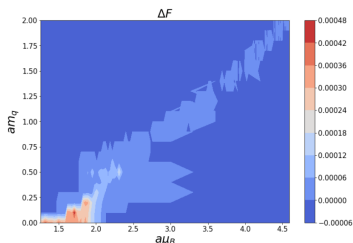


# Sign Problem of Dual Representation

Sign of a configuration  $C$  due to **geometry** of fermionic loops:

$$\sigma(C) = \prod_{\ell} \sigma(\ell), \quad \sigma(\ell) = (-1)^{1+w(\ell)+N_-(\ell)} \prod_{\tilde{\ell}} \eta_{\mu}(x)$$

- -1 for each fermion loop, each backward hopping (spatial or temporal), each winding number (anti-periodic bc); product of staggered phases  $\eta_{\mu}(x)$
- at strong coupling: mild residual sign problem  $\Delta_f \simeq 10^{-5}$ :
  - **baryons are heavy** (almost static)
  - color singlets closer to the **physical states** (hadrons)
  - no fluctuations from gauge fields (integrated out)!
- Sign problem in regime  $\beta = \frac{6}{g^2} \lesssim 1$  **mild enough** to study full phase diagram

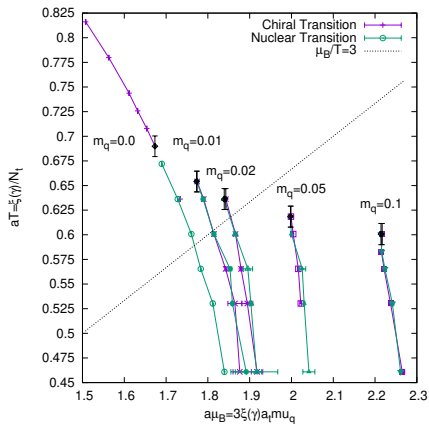
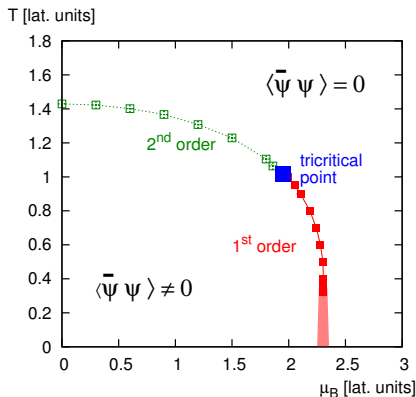


$\Delta_f$  at strong coupling as a function of  $m_q$      $\Delta_f$  in chiral limit as a function of  $\beta$

# The phase diagram in the strong coupling limit

Chiral and nuclear phase boundary obtained via Monte Carlo:

- at finite quark mass, the **tri-critical point** turns into  $Z_2$  critical end point
- chiral and nuclear first order lines also match at finite quark mass



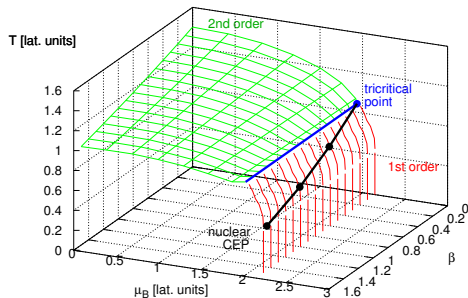
$\mu_q - T$  phase diagram in renormalized parameters [Kim & U. PoS Lattice 2016]

# Goal: What does the Phase Diagram including $\beta$ look like?

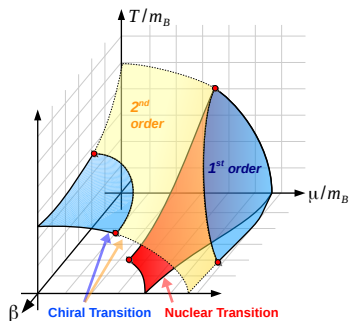
## Phase Diagram in the Strong Coupling Regime and Chiral Limit:

- Via **reweighting** in  $\beta$  from  $\beta = 0$ :  $\mathcal{O}(\beta)$  corrections for **SU(3)**

[Langelage, de Forcrand, Philipsen & U., *PRL* 113 (2014)]



[measured via Worm algorithm]



[one of several possible scenarios]

## Questions of interest:

- Do the **nuclear and chiral transition split?**
- Does the **tri-critical point** move to smaller or larger  $\mu$  as  $\beta$  is increased?

# Dualization of full lattice QCD

1 Combined **Taylor expansion** in the reduced gauge coupling  $\tilde{\beta} \equiv \frac{\beta}{2N} = \frac{1}{g^2}$  and quark mass  $\hat{m}_q$ , giving rise to **dual variables**:

$$n_p, \bar{n}_p, d_\ell, \bar{d}_\ell \text{ and } m_x:$$

$$\mathcal{Z}(\beta, \mu_q, \hat{m}_q) = \sum_{\{n_p, \bar{n}_p\}} \prod_p \frac{\tilde{\beta}^{n_p + \bar{n}_p}}{n_p! \bar{n}_p!} \prod_\ell \frac{1}{d_\ell! \bar{d}_\ell!} \prod_x \frac{(2\hat{m}_q)^{m_x}}{m_x!} \mathcal{G}_{n_p, \bar{n}_p, d_\ell, \bar{d}_\ell, m_x}$$

2 Evaluate 1-link integrals in  $\mathcal{G}$  in terms of **generalized Weingarten functions**

3 Decouple those integrals via a choice of orthogonal projectors:

4 Multi-indices  $\rho$  are new dual degrees of freedom: **decoupling operator indices**

5 Collect operators into a **local tensor**  $T_x^{\rho_x^d \dots \rho_x^x}$  that depends on participating dual degrees of freedom  $\mathcal{D}_x = \{m_x, d_{x, \pm\mu}, n_{x, \mu\nu}, \bar{n}_{x, \mu\nu}\}$

6 Final **dual partition function**:

$$\mathcal{Z}(\beta, \mu_q, \hat{m}_q) = \sum_{\{n_p, \bar{n}_p\}} \sum_{\{k_\ell, f_\ell, m_x\}} \sigma_f \sum_{\{\rho_{\pm\mu}^x\}} \prod_p \frac{\tilde{\beta}^{n_p + \bar{n}_p}}{n_p! \bar{n}_p!} \prod_{\ell=(x, \mu)} \frac{e^{\mu_q \delta_{\mu, 0} f_{x, \mu}}}{k_\ell! (k_\ell + |f_\ell|)!} \prod_x \frac{(2\hat{m}_q)^{m_x}}{m_x!} T_x^{\rho_x^d, \dots, \rho_x^x}(\mathcal{D}_x)$$

[G. Gagliardi & W. U. PRD 101, (2020) 034509]

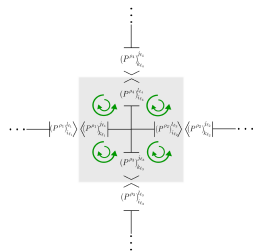
**Truncation at  $\mathcal{O}(\beta^2)$ :** allow for plaquette occupations  $(n_p, \bar{n}_p) \in \{(1, 1), (2, 0), (0, 2)\}$  7

# Monte Carlo for TN-Representation via Vertex Model

- Each tensor can be transformed into a vertex:  
DOI  $\rho_b^x$  per bond cast into integers  
vertex weight depends on directions

- Number of distinct vertices (SU(3),  $d = 4$ )

limit	$\mathcal{O}(\beta^0)$	$\mathcal{O}(\beta^1)$	$\mathcal{O}(\beta^2)$	$\mathcal{O}(\beta^3)$
all	221	3485	51125	681013
chiral	176	2960	<b>44672</b>	607792
quenched	1	1	25	137

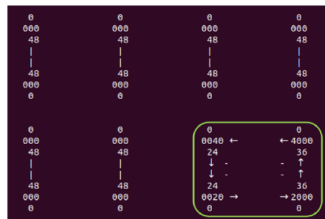


- compare to 8-vertex model for SC U(1),  
 $d = 2$  [U. Wenger PRD 80 (2009) 071503]
- Some vertices have negative weight, but most configurations are positive
- Use **heatbath algorithm** for to modify vertices along closed contours; has been parallelized; Worm algorithm not yet applicable beyond  $\mathcal{O}(\beta)$

[P. Pattanaik & U. PoS Lattice (2023)]

- At  $\mu_B = 0$ : crosschecked with HMC

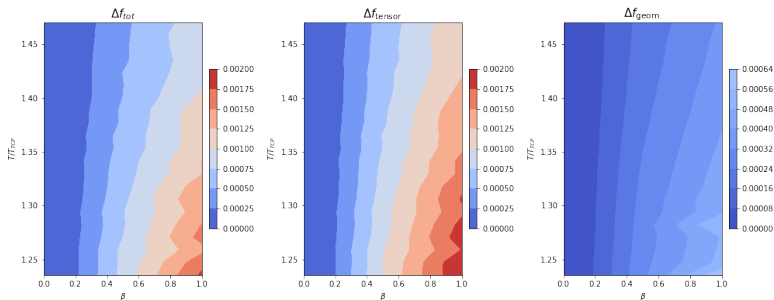
- Lattice Setup:  $8^3 \times 4$ ,  $12^3 \times 4$  and  $16^3 \times 4$ , SC, and  $\mathcal{O}(\beta)$ ,  $\mathcal{O}(\beta^2)$  for  $\beta = [0.0, \dots, 1.0]$  and at  $T = 0.8, 0.85, 0.9, 0.95, 1.0$ , all for chiral limit





# Sign Problem of Vertex Formulation

- In addition to the geometric fermionic sign  $\sigma_{\text{geom}}(C)$ , also the tensors  $T_x^p$ /vertices  $v_x$  can be negative:  $\sigma_{\text{tot}}(C) = \sigma_{\text{tensor}}(C)\sigma_{\text{geom}}(C)$ ,  $\sigma_{\text{tensor}}(C) = \prod_x v_x^i$
- This particularly worsens the sign problem for  $\mathcal{O}(\beta^2)$ , where non-trivial decoupling operator indices are present
- Additional tensor sign results in larger statistical errors for  $\mathcal{O}(\beta^2)$  up to  $\beta \lesssim 1$
- Finite size scaling for  $\mathcal{O}(\beta^2)$  remains difficult

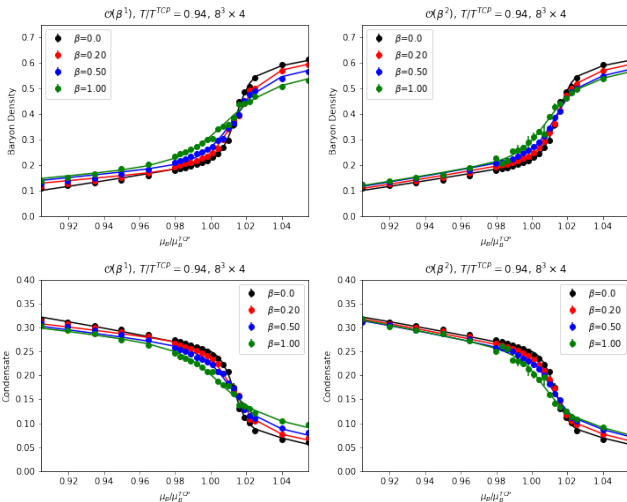


*Decomposition:  $\Delta f_{\text{tot}} = \Delta f_{\text{tensor}} + \Delta f_{\text{geom.}}$ , data for  $\mu_B/\mu_B^{\text{TCP}} = 0.75, 8^3 \times 4$*

# Results: Baryon Density and Chiral Condensate

- All results relative to the location of the strong coupling tricritical point:

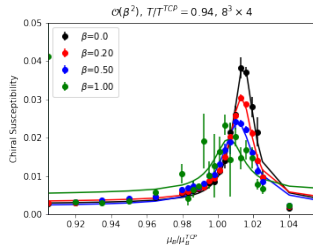
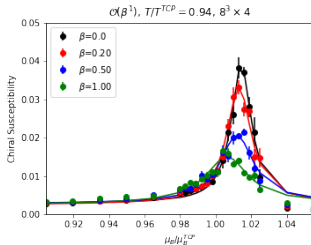
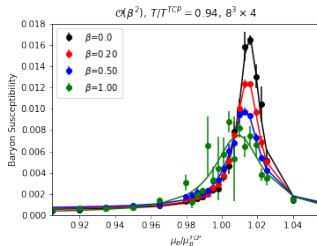
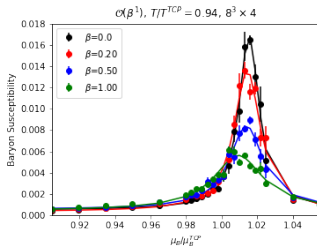
$$T_{N_\tau=4}^{TCP} = 0.85, \mu_B^{TCP} = 1.99$$



# Results: Baryon Susceptibility, Chiral Susceptibility

- All results relative to the location of the strong coupling tricritical point:

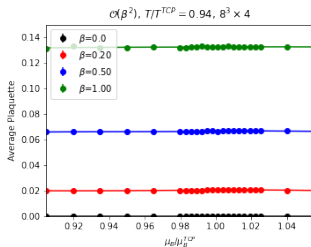
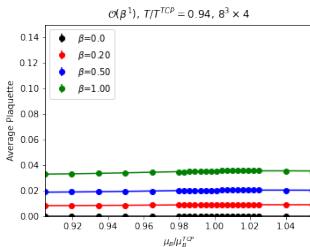
$$T_{N_\tau=4}^{TCP} = 0.85, \mu_B^{TCP} = 1.99$$



## Results: Average Plaquette

- All results relative to the location of the strong coupling tricritical point:

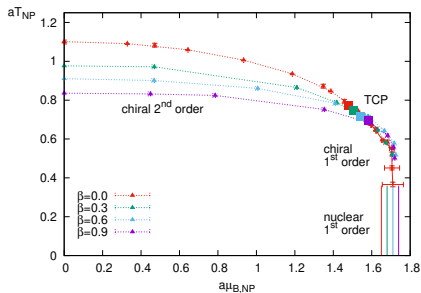
$$T_{N_\tau=4}^{TCP} = 0.85, \mu_B^{TCP} = 1.99$$



- Average plaquette and its susceptibility: no imprint of the chiral/nuclear transition

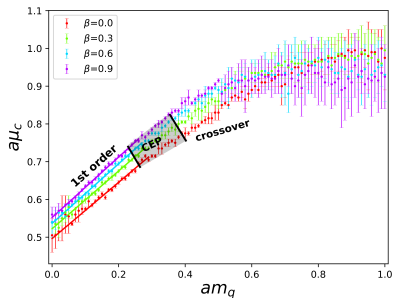
# Phase Diagram in the Strong Coupling Regime $\beta > 0$

## Phase Diagram in Chiral Limit:



- taking into account the  $\beta$ -dependent renormalization of  $aT$  and  $a\mu_B$
- **tri-critical point** depends only slightly on  $\beta$

## $m_q$ -Dependence of Nuclear Transition:



- **weak  $\beta$ -dependence of transition  $\mu_c(m_q)$**  at fixed  $T \simeq 0$
- consistent with findings of other results (Meanfield, 3d-effective theory)
- location of nuclear CEP challenging

## Prospects for the strong coupling expansion

- Higher orders  $\mathcal{O}(\beta^n)$  with  $n > 2$  may not be required for  $\beta \lesssim 1$
- Continuum physics expected to emerge above  $\beta \sim 2N_c$   
 → Large plaquette occupation numbers ( $n_p, \bar{n}_p$ ) cannot be neglected.
- For  $\beta > 1$ : instead of Taylor expansion, a character expansion would have to be established (for staggered fermions: so far only a posteriori identified):

$$\prod_p \exp \frac{\beta}{2N_c} (\text{Tr} U_p + \text{Tr} U_p^\dagger) = \prod_p \sum_\lambda u_\lambda(\beta/N_c) \chi_\lambda(U_p)$$

but with staggered fermions on top

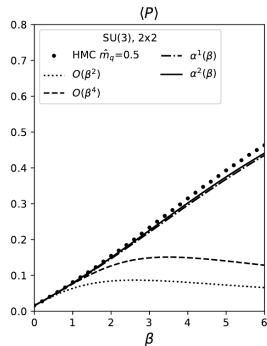
- Recursive relations for  $SU(3)$  via 3-step Lucas Polynomials, resulting in

$$\chi_\lambda(U_p) = \sum_{n_p, \bar{n}_p} c_\lambda(n_p, \bar{n}_p) \text{Tr}[U_p]^{n_p} \text{Tr}[U_p^\dagger]^{\bar{n}_p}$$

$$\alpha_{n_p, \bar{n}_p}^r(\beta) \equiv \sum_{\{\lambda\}_r} c_\lambda(n_p, \bar{n}_p) u_\lambda(\beta/3),$$

neglecting all  $\lambda = (\lambda_1, \dots)$  with  $\lambda_1 > r$

- Sign problem would kick in at larger  $\beta$



*Taylor vs. character expansion*

# Quantum Simulations on a Quantum Annealer

- Quantum Annealer (D-Wave): array of qubits modeled by quantum spin glass  $H_{\text{Ising}}$ , with annealing process given by transverse external field:

$$H(s) = -A(t) \sum \sigma_x^i + B(t) H_{\text{Ising}}$$

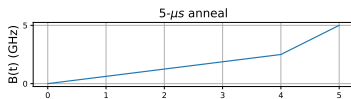
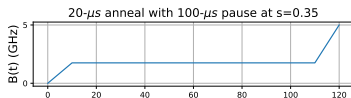
- Minimization: find optimal **binary solution vector**  $x$

$$\chi^2 = x^T W x + p \|Ax + b\|^2 = x^T Q x + C,$$

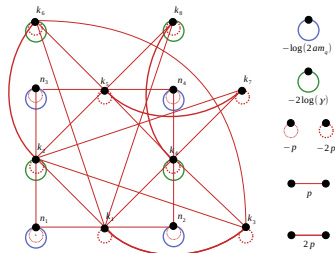
with QUBO (Quadratic Unconstrained Binary Optimization) matrix:

$$Q = W + p (A^T A + \text{diag}(2b^T A)), \quad C = p b^T$$

with weight matrix  $W$ , constraint  $(A, b)$  and the penalty factor  $p$



Annealing profile given by  $B(t)$



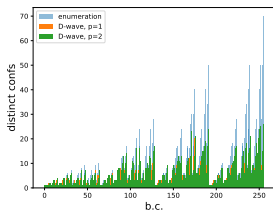
Problem Graph implementing QUBO matrix

# D-Wave Simulations for Strong Coupling LQCD

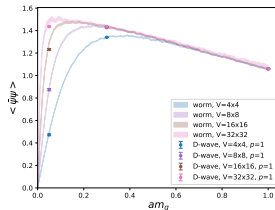
- For SC-LQCD: Demonstrated that it implements **importance sampling**

[J. Kim, T. Luu, U. PRD 108 (2023)]

- Particularly useful at **low  $T$** , where classical algorithms are expensive
- Large volumes addressed via histograms  $h$  obtained from D-Wave for  $2 \times 2$  sub-lattices with fixed boundaries, iterating in parallel through sub-lattices
- Histograms approximate well true distribution for  $p = 1$ ,
- Use hybrid strategy with Metropolis-Hastings  $P_{\text{accept}} = e^{-S_{\text{new}} + S_{\text{old}}} \frac{h_{\text{old}}}{h_{\text{new}}}$  to improve on validity rate and acceptance rate



Number of histogram entries per boundary condition



Comparing results from D-Wave and Worm algorithm

[J. Kim, T. Luu, U. arXiv:2412.11677]

- Results at  $\mathcal{O}(\beta)$  for  $SU(3)$  are underway, Metropolis-Hastings still feasible.



## Gate-based Quantum Simulations for SCE: Preliminaries

- Quantum annealers not flexible enough to address important aspects of a Hamiltonian
- Usual Hamiltonian approach to quantum simulations of LGTs: KS-Hamiltonian

$$\mathcal{H}_{\text{KS}} = \frac{1}{2a} \left( g^2 \sum_{\ell \in \text{Links}} E_{\ell} E_{\ell} + \frac{1}{g^2} \sum_{\rho \in \text{Plaquettes}} \text{Tr}[2\mathbb{1} - P_{\rho} + P_{\rho}^{\dagger}] \right)$$

( $A_0 = 0$ , operators in electric basis, Hilbert space must be truncated, different charge sectors )

- Hamiltonian derived from SCE at fixed order: Occupation number basis, everything discrete from the start  
→ Hilbert space remains **finite-dimensional**
- No further truncation of Hilbert space needed
- Grassmann constraint and Gauss's law respected implicitly
- So far: no actual quantum simulations yet, emulation via `qiskit`

# Euclidean Continuous Time Limit

Continuous time (CT) methods:

- make time direction continuous:  $t \in [0, \beta]$ ,  
sample  $Z(\beta)$  in terms of **decay probabilities**  
[Beard & Wiese, PRL 77 (1996) 5132] (for AFHM)

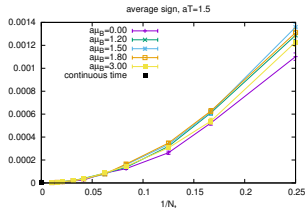


For Strong Coupling LQCD:

- Introduce **bare anisotropy**  $\gamma$  such that  $\xi = \frac{a_s}{a_t} \neq 1$ :
- Non-perturbative result:  $\xi(\gamma) \approx \kappa\gamma^2 + \frac{\gamma^2}{1+\lambda\gamma^4}$ ,  $\kappa = 0.781(1)$   
[de Forcrand, Vairinhos, U., PRD 97 (2018)]
- Define the **continuous Euclidean time limit** (CT-limit):

$$N_\tau \rightarrow \infty, \quad \xi, \gamma \rightarrow \infty, \quad aT = \frac{\xi(\gamma)}{N_\tau} \simeq \kappa\mathcal{T}(\gamma, Nt), \quad \mathcal{T} = \frac{\gamma^2}{N_\tau} \text{ fixed}$$

- **only one parameter**  $\mathcal{T}$
- non-perturbative factor  $\kappa$  directly in CT-limit!
- baryons are heavy:  $\Delta f \simeq 10^{-5}$
- in continuous time limit  $N_\tau \rightarrow \infty$ :  
**baryons become static**  
 $\Rightarrow$  finite density sign problem absent!

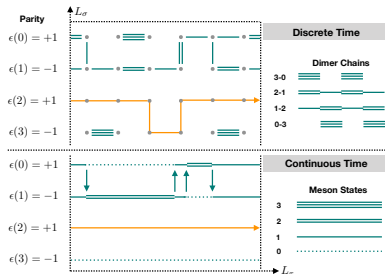


$\Delta f$  vanishes for  $N_\tau \rightarrow \infty$  ( $a_t \rightarrow 0$ )

# From Meson Occupation Numbers to Hamiltonian ( $N_f = 1$ )

Correspondence between discrete and continuous time:

- alternating dimer chains (top) and **meson occupation numbers  $m$**  (bottom):
- multiple spatial dimers become **resolved in single spatial dimers**, oriented consistently due to even-odd ordering
- **conservation law**: for mesons connecting  $\langle x, y \rangle$



$$m_x \mapsto m_x \pm 1 \quad \Leftrightarrow \quad m_y \mapsto m_y \mp 1$$

Derive Hamiltonian via **diagrammatic expansion** of  $Z_{CT} = \lim_{\gamma, N_T \rightarrow \infty} Z_{N_T}(\gamma)$

- express the partition function as series in inverse temperature  $\frac{1}{T} = \frac{N_T}{\gamma^2}$ :

$$Z_{CT}(\mathcal{T}, \mu_B) = \text{Tr}_b \left[ e^{(\hat{\mathcal{H}} + \hat{\mathcal{N}} \mu_B) / \mathcal{T}} \right], \quad \hat{\mathcal{H}} = \frac{1}{2} \sum_{\langle \vec{x}, \vec{y} \rangle} (\hat{J}_{\vec{x}}^+ \hat{J}_{\vec{x}}^- + \hat{J}_{\vec{x}}^- \hat{J}_{\vec{x}}^+), \quad \hat{\mathcal{N}} = \sum_{\vec{x}} \hat{\omega}_{\vec{x}}$$

# Quantum Hamiltonian: Creation and Annihilation Operators

**Creation**  $\hat{J}^+$  and **annihilation operators**  $\hat{J}^- = (\hat{J}^+)^T$ :

- contain the matrix elements  $\langle m_1 | 1 | m_2 \rangle$  with  $\hat{v}_L = \langle 0 | 1 | 2 \rangle = 1$ ,  
 $\hat{v}_T = \langle 1 | 1 | 1 \rangle = \frac{\sqrt{3}}{4}$ :

$$\hat{J}^+ = \left( \begin{array}{cccc|cc} 0 & 0 & 0 & 0 & 0 & 0 \\ \hat{v}_L & 0 & 0 & 0 & 0 & 0 \\ 0 & \hat{v}_T & 0 & 0 & 0 & 0 \\ 0 & 0 & \hat{v}_L & 0 & 0 & 0 \\ \hline & & & & 0 & 0 \\ & & & & 0 & 0 \end{array} \right), \quad \hat{\omega} = \left( \begin{array}{cccc|cc} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \hline & & & & 1 & 0 \\ & & & & 0 & -1 \end{array} \right)$$

- **local Hilbert space** per site:  $|h\rangle = |m, b\rangle \in \mathbb{H}_h = [0, \pi, 2\pi, 3\pi; B^+, B^-]$
- block-diagonal structure due to vanishing commutator  $[\hat{\mathcal{H}}, \hat{\mathcal{N}}] = 0$

Interpretation (generalized to  $N_c \geq 3$ ):

- **pion current is conserved**
- Pauli saturation on the level of quarks as hadrons have fermionic substructure  
 $\rightarrow |m\rangle$  bounded from above,  $m \mapsto s = m - \frac{N_c}{2}$   
 $\rightarrow$  **particle-hole symmetry**,  $N_c + 1$ -dim. irrep of  $SU(2)$ :

$$\hat{J}_1 = \frac{\sqrt{N_c}}{2} (\hat{J}^+ + \hat{J}^-), \quad \hat{J}_2 = \frac{\sqrt{N_c}}{2i} (\hat{J}^+ - \hat{J}^-), \quad \hat{J}_3 = \frac{N_c}{2} [\hat{J}^+, \hat{J}^-], \quad \hat{J}^2 = \frac{N_c(N_c + 2)}{4}$$

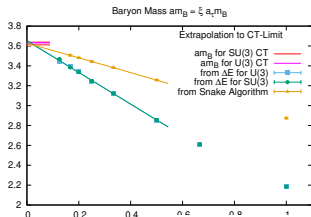
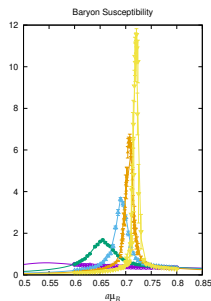
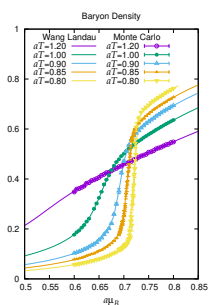
$$\hat{J}_3 \left| \frac{N_c}{2}, s \right\rangle = s \left| \frac{N_c}{2}, s \right\rangle, \quad \hat{J}^2 \left| \frac{N_c}{2}, s \right\rangle = \frac{N_c(N_c + 2)}{4} \left| \frac{N_c}{2}, s \right\rangle, \quad [\hat{J}^2, \hat{J}_3] = 0.$$

# Quantum Monte Carlo for $N_f = 1$ Hamiltonian, Results

QMC is a continuous time **Worm algorithm**:

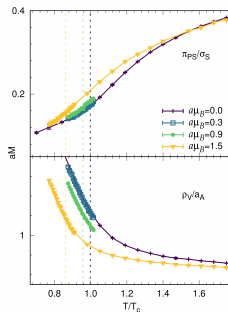
- Temporal locations uniformly distributed according to a **Poisson process**:

$$P(\Delta t) = e^{-\lambda \Delta t}, \quad \Delta t \in [0, 1], \quad \lambda \text{ is the "decay constant" for pion exchange}$$



- Baryon mass could be unambiguously determined
- **meson pole masses** can be extracted from the Euclidean time correlators for various spin kernels
- pion mass  $M_\pi$  **sensitive to chiral transition**

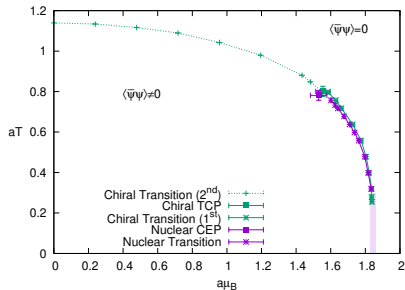
[Klegrew, U. PRD 102 (2020)]



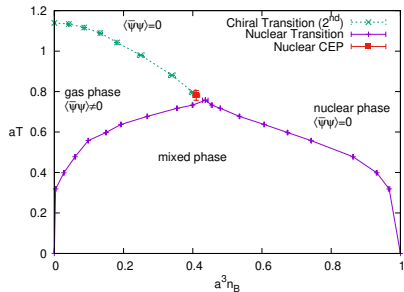
# Phase Diagrams from $N_f = 1$ Hamiltonian LQCD (Chiral Limit)

From **Quantum Monte Carlo** / Density of States Method:

- obtain baryonic observables and phase diagrams to high precision



Grand-canonical phase diagram



Canonical phase diagram

[Klegrewe, U. PRD 102 (2020)]

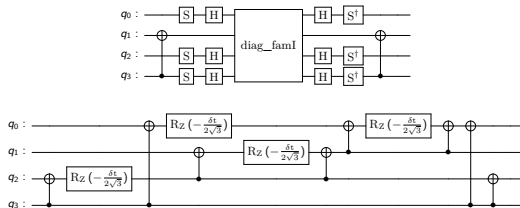
# Gate-based Quantum Computing: Circuits

To identify the gate set required for quantum simulations ( $N_f = 1$ ):

- Qubitize the Hamiltonian  $\mathcal{H}$  in mesonic and baryonic sector independently:  
 $|h\rangle_x = |m\rangle_x \oplus |b\rangle_x$ , 2 qubits for mesons, 1 control qubit for baryons
- Partition  $\mathcal{H}_{meson}$  into mutually commuting even/odd parts and decompose each into **Pauli strings** (with  $c_i$  depending on  $\hat{v}_L$  and  $\hat{v}_T$ ):

$$\mathcal{H} = \sum_{x_e} \mathcal{H}_{x_e} + \sum_{x_o} \mathcal{H}_{x_o}, \quad \mathcal{H}_{x_{e/o}} = \sum_i c_i P_i, \quad P_i \in \{I, X, Y, Z\}^{\otimes(2+2)}$$

- Four families of Pauli strings, e.g.  $\text{Fam}_1 = \{(IX)_x(YY)_y, (IY)_x(YX)_y + x \leftrightarrow y\}$

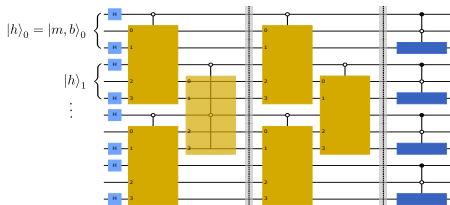


*Top: four qubit quantum gate corresponding to  $\text{Fam}_1$ .*

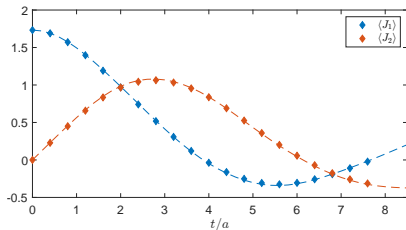
*Bottom: diagonal gate of the above unitary, decomposed into elementary operations.*

# Gate-based Quantum Computing: Emulation

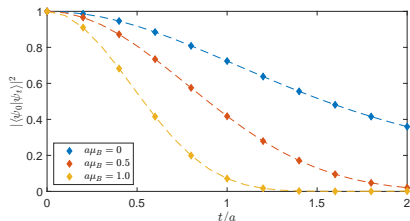
- Trotterized time evolution in 1+1 dimension,  $L = 4$



Mesonic Trotter steps (yellow) and baryonic evolution (blue)



Mesonic  $\hat{J}_1$ ,  $\hat{J}_2$ , exact results versus simulated with Trotter step size  $\delta_t = 0.4$



Wave function overlap for various  $\mu_B$  with Trotter step size  $\delta_t = 0.2$



## Partition Function: $N_f > 1$

**Local Hilbert space**  $\mathbb{H}_h$  via canonical sectors  $B \in [-N_f, -N_f + 1, \dots, N_f]$ :

- $\mathbb{H}_h$  quickly grows with  $N_f$ , general formula: [U., Lattice 2014]:

$$Z_{\text{stat}}(N_c, N_f) \sum_{B=-N_f}^{N_f} \prod_{a=0}^{N_c} \frac{a!(2N_f + a)!}{(N_f + a + B)!(N_f + a - B)!} e^{B\mu_B/T}$$

- coefficient encodes number of **hadronic states**  $h$ , for gauge group  $SU(3)$ :
  - $N_f = 2$ :  $d = [1, 20, 50, 20, 1] = 92$
  - $N_f = 3$ :  $d = [1, 56, 490, 980, 490, 56, 1] = 2074$

Every state of the local Hilbert space can be described by a **set of charges**:

- $B \in \{-N_f, \dots, N_f\}$ ,  $I \in \{-N_c, \dots, N_c\}$ ,  $U, D \in \{0, \dots, N_c\}$  for  $N_f = 2$
- $K_1, K_2 \in \{-N_c, \dots, N_c\}$ ,  $S \in \{0, \dots, N_c\}$  additionally for  $N_f = 3$

## Quantum Hamiltonian for $N_f = 2$

The Hamiltonian has  $N_f^2$  contributions, one for each pseudoscalar meson:

- Partition function for  $N_f = 2$ :

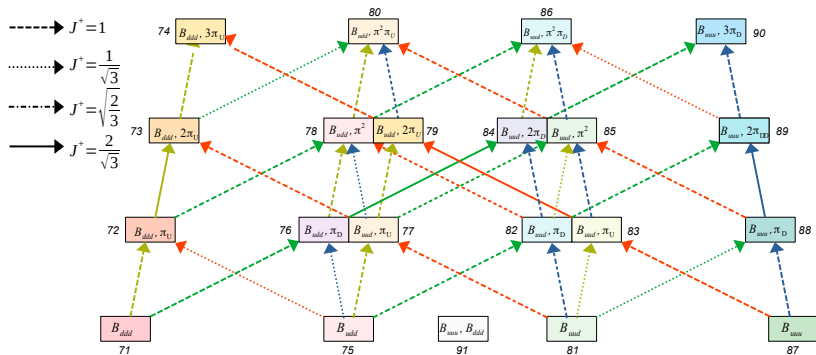
$$Z_{\text{CT}}(\mathcal{T}, \mu_B, \mu_I) = \text{Tr}_{\mathfrak{h}} \left[ e^{(\hat{\mathcal{H}} + \hat{\mathcal{N}}_B \mu_B + \hat{\mathcal{N}}_I \mu_I) / \mathcal{T}} \right] \quad \mathfrak{h} \in \mathbb{H}_{\mathfrak{h}}$$
$$\hat{\mathcal{H}} = \frac{1}{2} \sum_{\langle \vec{x}, \vec{y} \rangle} \sum_{Q_i \in \{\pi^+, \pi^-, \pi_U, \pi_D\}} (\hat{J}_{Q_i, \vec{x}}^+ \hat{J}_{Q_i, \vec{y}}^- + \hat{J}_{Q_i, \vec{x}}^- \hat{J}_{Q_i, \vec{y}}^+)$$

- For the transition  $\mathfrak{h}_1 \mapsto \mathfrak{h}_2$ , the **matrix elements**  $\langle \mathfrak{h}_1 | Q_i | \mathfrak{h}_2 \rangle$  of  $\hat{J}_{Q_i}^{\pm}$  are determined from Grassmann integration and diagonalization
- Only non-zero which are consistent with current conservation of all  $Q_i$ ,  
**and turn out to be positive!**  
(Note: that requires the Euclidean continuous time limit, while for finite  $N_{\tau}$  there remain negative weights for  $N_f > 1$ )
- Again,  $[\mathcal{H}, \hat{\mathcal{N}}_B] = 0$ , however  $[\mathcal{H}, \hat{\mathcal{N}}_I] \neq 0$



# Hadronic States for $N_f = 2$

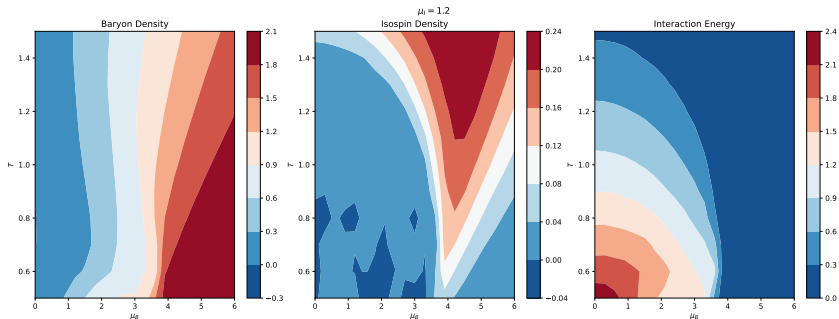
Transitions according to  $J^+$ , quantum numbers  $B = 1, I = -3/2, \dots, 3/2, m = 0 \dots 3$   
and  $B = 2, I = 0, m = 0$



## Preliminary Results for $N_f = 2$ CT-Worm simulations

$N_f = 2$  allows to study SC-LQCD at both **finite baryon and isospin density**:

- enlarged  $\mu_B - \mu_I - T$  phase diagram accessible
- Mean-field predicts: both the nuclear and chiral transition split up into two transitions as  $\mu_I > 0$ , first indications from MC simulations: with increasing  $\mu_I$ , the plateau between the two transitions increases (lower  $T$  required)



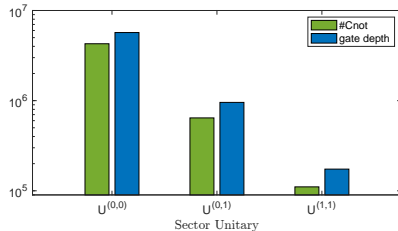
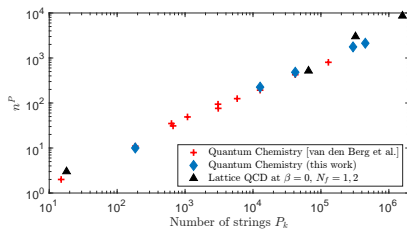
*Contour plots of nuclear, isospin and chiral observables in the  $\mu_B - T$  plane for  $\mu_I = 1.2$*

New physics expected:

- single baryons can coexist with pions  $\rightarrow$  **pion exchange** between nucleons
- **pion condensation** competes with nuclear phase

# Prospects for Quantum Chemistry Simulations for $N_f = 2$

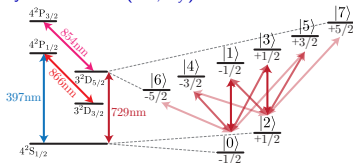
- Hilbert space 92-dimensional, 9 qubits required
- Too complex to determine minimal set of commuting families of Pauli strings
- With qubits: **high gate depth** for single Trotter step
- Time evolution of baryonic sectors mix (meson exchange for  $B = 0, \pm 1$ )



Number of partitions as a function of the number of Pauli strings

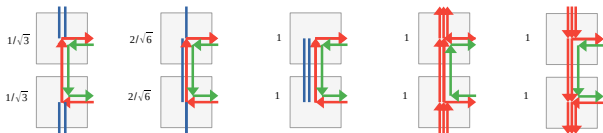
Number of entangled CNOT gates, gate depth in baryonic sectors ( $B_x, B_y$ )

- Less complexity: qudits ( $d$ -level systems): each  $U$  an elementary operation
- With trapped ions, e.g.  $^{40}\text{Ca}$ : 8 levels
- Entangled gate count:  $nn$ ,  $N_f = 2$ ,  $d > 2$ :  $\mathcal{O}(10^6)$  qubits  $\mapsto \mathcal{O}(10^2)$  qudits



## Prospects for Quantum Simulations for $\beta > 0$

- At finite temperature: spatial plaquettes are suppressed over temporal plaquettes
- In the continuous time limit: only **temporal plaquettes** survive



- Temporal plaquettes are of same order as meson exchange, but also allows to **couple to baryons!** ( $\hat{J}^\pm$  still block-diagonal for  $N_f = 1$ ):

$$J^+ = \left( \begin{array}{cccc|cc} v_{M,0} & 0 & 0 & 0 & 0 & 0 \\ v_L & v_{M,1} & 0 & 0 & 0 & 0 \\ 0 & v_T & v_{M,2} & 0 & 0 & 0 \\ 1 & 0 & v_L & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & v_B & 0 \\ 0 & 0 & 0 & 0 & 0 & v_B \end{array} \right), \quad v_{M,0} = \frac{1}{3g}, \quad v_{M,1} = \frac{2}{3g}, \quad v_{M,2} = \frac{1}{g},$$

$$v_B = \frac{1}{g}, \quad v_B = \frac{1}{g}.$$

- General SCE: Enlarged but **still finite Hilbert space**:  
(anti-) quarks  $d_I, \bar{d}_I = 0, \dots, N_c$  vary independently: 16-dimensional for  $N_c = 3$
- Still NN interaction  $J^+ J^-$ , requiring  $4 \times 4$  qubit coupling
- Caveat: Spatial plaquettes would enlarge Hilbert space further, no longer NN

# Conclusions

## Summary:

- Dual representation that is in principle not truncated in  $\beta$  established, caveat: it re-introduces the sign problem gradually with  $\beta$
- TCP remains invariant when comparing  $\mathcal{O}(\beta)$  and  $\mathcal{O}(\beta^2)$
- Nuclear transition at  $\mathcal{O}(\beta)$  has small  $\beta$ -dependence
- Hamiltonian formulation based on CT-limit **sign problem-free** for  $N_f = 1, 2, 3$
- Matrix elements for the **creation and annihilation operators**  $\hat{J}^\pm$  have now been determined for  $N_f = 2$  and for  $\mathcal{O}(\beta)$
- First exploratory  $N_f = 2$  QMC simulations at  $\mu_B > 0$ ,  $\mu_I > 0$  (lower  $T$  required)
- Strong coupling LQCD on a quantum annealer allows very low  $T$
- Gate-based quantum computing feasible for  $N_f = 1$ , not yet feasible for  $N_f = 2$  (huge QC resources required)

If TCP remains invariant for higher orders in  $\beta$ : CEP also exists in the continuum!